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Karl Christe (ERC) et al., "Nitrogen Fluoride Chemistry" (abstract)

↳ 55194 (unofficial notification)

ACS Meeting

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(Statement A)

Dr. Carley  
55881

## Nitrogen Fluoride Chemistry

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The isomerization of trans-N<sub>2</sub>F<sub>2</sub> to cis-N<sub>2</sub>F<sub>2</sub> going through N<sub>2</sub>F<sup>+</sup>AsF<sub>6</sub><sup>-</sup> is unpredictable, erratic, requires 2 steps, and consumes an equimolar amount of AsF<sub>5</sub>. It was found that catalytic amounts of SbF<sub>5</sub> at 30C can achieve this isomerization, but still result in substantial N<sub>2</sub>F<sub>2</sub> losses due to N<sub>2</sub>F<sup>+</sup>SbF<sub>6</sub><sup>-</sup> formation. When the reaction is carried out at 60C, surprisingly NF<sub>4</sub><sup>+</sup>SbF<sub>6</sub><sup>-</sup>.nSbF<sub>5</sub> is formed. The crystal structures of N<sub>2</sub>F<sup>+</sup>SbF<sub>6</sub><sup>-</sup> (disordered), N<sub>2</sub>F<sup>+</sup>SbF<sub>6</sub><sup>-</sup> (disordered), N<sub>2</sub>F<sup>+</sup>Sb<sub>2</sub>F<sub>11</sub><sup>-</sup> (ordered), and NF<sub>4</sub><sup>+</sup>Sb<sub>2</sub>F<sub>11</sub><sup>-</sup> were determined and are discussed. AlF<sub>3</sub> was also studied as a catalyst for the N<sub>2</sub>F<sub>2</sub> isomerization and was found to be an ideal catalyst resulting in very high conversions of trans-N<sub>2</sub>F<sub>2</sub> and high yields of cis-N<sub>2</sub>F<sub>2</sub>. The AlF<sub>3</sub> can be used repeatedly without loss of activity or N<sub>2</sub>F<sup>+</sup> salt formation. Cis-N<sub>2</sub>F<sub>2</sub> forms with SnF<sub>4</sub> at low temperatures a 2:1 salt, (N<sub>2</sub>F<sup>+</sup>)<sub>2</sub>SnF<sub>6</sub><sup>2-</sup>, that slowly loses N<sub>2</sub>F<sub>2</sub> at room temperature to give N<sub>2</sub>F<sup>+</sup>SnF<sub>5</sub><sup>-</sup>. The crystal structure of H<sub>3</sub>NF<sup>+</sup>CF<sub>3</sub>SO<sub>3</sub><sup>-</sup> was also determined and exhibits a relatively long N-F bond.

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